

Nonuniversal properties of the single-particle density of states of 1D system with electron-phonon interactions

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We have calculated the single-particle density of states (DOS) for a model of spinfull Tomonaga-Luttinger liquid with frequency dependent parameter K_c of the charge sector (and $K_s = 1$ of spin sector). Such frequency dependence may originate from interactions with optical phonons. DOS exhibits a power-law suppressed asymptotic behaviour near $\omega = 0$ with exponent larger than one, in agreement with previous results. For larger frequencies, but still not far away from the origin, DOS exhibits a peak, the position of which scales as $[K(0) + K^{-1}(0)]\omega_0$, where ω_0 is the characteristic phonon frequency. The position of the peak decreases as the phonon's frequency becomes smaller. It is interesting that the peak of DOS does not coincide with the characteristic phonon frequency.

This paper investigates the properties of the single-particle density of states (DOS) at the Fermi surface of 1D conductors with electron-electron and electron-phonon interactions. Interest in the problem of the electron-phonon 1D systems has been motivated mainly by many interesting results on organic conductors and superconductors, conducting polymers and also photoemission experiments on the properties of the spectral function near the fermi surface [1], which are known to be influenced strongly by the electron-phonon coupling. The electron-phonon interaction in quasi-one dimensional materials has been studied by different authors, but mostly for the case of the noninteracting electrons [2–5]. Here the effects of interaction of the charge density with small momentum phonons were treated and the direct diagonalization of the Hamiltonian could be done. The combined effects of Coulomb and electron-phonon interactions for phonons with finite frequencies was studied in the case of spinless fermions by [6] and the spinfull case by the same authors [7]. In these papers the effects of dispersionless phonons with momenta $\approx 2k_F$ were investigated. In both cases the renormalization group approach was used. The effort on those papers was concentrated, however, on the effective interaction constants, effective mass due to electron-phonon coupling and renormalized velocities for the charge and spin flucuations. A possible phase diagram (in presence of suitable coupling mechanisms between chains) was represented.

In this paper we consider the effects of electron-phonon, in addition to electron-electron interactions, in the framework of Tomonaga-Luttinger liquid model. We focus on large momentum transfer scatterings, of $q \approx 2k_F$, $q \approx 4k_F$, of electrons by phonons. The electron-electron part of the Hamiltonian [Eq. (2) below] can be written as a sum of two independent (commuting) contributions of charge and spin collective modes. To count for the phonons, in the continuous description, we separate in fast and slow components the deformation field of the lattice sites. We keep only the components near $2k_F$ and $4k_F$ of this field. Physically the $2k_F$ component interacts with electrons in which one electron hopes from one Fermi point to the other. Similarly the $4k_F$ component interacts with electrons and now two electron can hope from one Fermi point to the other. We integrate out the phonon degrees of freedom and examine the remaining effective electron-electron interactions. The electron-phonon interaction, as observed also in the papers cited above, affects the charge as well as the spin sector by renormalizing the coupling constant g_s and the Tomonaga-Luttinger liquid parameter of the charge sector K_c . The study here is confined to the case when g_s remains negative, i.e. on the case of gapless spin excitations. Our approach is similar to the one of Voit and Schulz [6,7], but we differ on the way we treat the retardation effects appearing from the presence of the electron-phonon interactions. In [6,7] they use a perturbative expansion to study the retardation effects whereas we investigate their effects by studying the effective Luttinger liquid to which the electron-phonon interactions give rise to the frequency dependend parameter K_c of the charge sector. We find the imaginary time single particle Matsubara Green's function and numerically produce the single-particle density of states of this unusual Luttinger liquid.

The model we consider is the one-dimensional (1D) Hubbard model coupled to phonons. The lattice effects can be included in this model by making the hopping integral t dependent on the intercite distance:

$$t_{ij} \approx t + \frac{1}{2a}\kappa(u_i - u_j) . \quad (1)$$

This has been proposed for the first time by Su, Schrieffer and Heeger [8] to describe the physics of conducting polymers. The Hamiltonian with the above hopping integral has the following form:

$$H = -t \sum_{j,\sigma} (c_{j+1,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + U \sum_j n_{j\uparrow} n_{j\downarrow} - \frac{1}{2a} \kappa \sum_{j,\sigma} (u_j - u_{j+1}) (c_{j+1,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + H_{\text{ph}} , \quad (2)$$

where u_j is dimensionless and κ has dimensions of energy. The $c_{j,\sigma}$ operators are the usual creation and annihilation operators for the electrons with spin σ in the Wannier orbitals at site j and $n_{j,\sigma}$ is the number of electrons on site j . U is the repulsion of two electrons on the same site. We consider here the case of the incommensurate band filling i.e. $4k_F \neq 2\pi/a$, and therefore we do not consider umklapp scattering.

Substituting the creation and annihilation operators in terms of the new continuous fields $R_\sigma(x), L_\sigma(x)$, and introducing the scalar U(1) and vector SU(2) currents $J =: L_\alpha^\dagger L_\alpha :$, $\mathbf{J} =: L_\alpha^\dagger (\vec{\sigma}_{\alpha,\beta}/2) L_\beta :$, the first term of (2) can be written as a sum $H_1 = H_1^{U(1)} + H_1^{SU(2)}$. Adding to the above part of the Hamiltonian the U -interaction term one has $H_{\text{Hubb}} = H_c + H_s$, where

$$H_c = \frac{\pi \bar{v}_c}{2} \int dx (JJ + \bar{J}\bar{J}) + g_c \int dx J\bar{J} \quad , \quad H_s = \frac{2\pi \bar{v}_s}{3} \int dx (\mathbf{J}\mathbf{J} + \bar{\mathbf{J}}\bar{\mathbf{J}}) + g_s \int dx \mathbf{J}\bar{\mathbf{J}} \quad , \quad (3)$$

with Fermi velocities $\bar{v}_c = v_F(1 - Ua/(8\pi v_F))$ and $\bar{v}_s = v_F(1 - 9Ua/(8\pi v_F))$ and coupling constants $g_c = Ua/2$, $g_s = -2Ua$, in the charge and spin sectors respectively. The coupling constant in the spin sector is negative which results in the spin excitations being gapless (the $g_s \mathbf{J}\bar{\mathbf{J}}$ term is marginally irrelevant in the case g_s is negative). Using Abelian bosonization one can restore to H_c given by (3) the canonical Gaussian form:

$$H_c = \frac{v_c}{2} \int dx \left[K_c^0 \Pi_c^2 + \frac{1}{K_c^0} (\partial_x \Phi_c)^2 \right] \quad , \quad (4)$$

whith v_c and K_c^0 depending on the coupling constant g_c in the following way: $v_c = \bar{v}_c(1 - g_c^2/\pi^2 \bar{v}_c^2)^{1/2}$ and $K_c^0 = [(1 - g_c/\pi \bar{v}_c)/(1 + g_c/\pi \bar{v}_c)]^{1/2}$. We will see that the electron phonon interactions lead particularly to strong renormalization of the parameters of the charge sector.

The effect of electron-phonon interactions on the dynamics of the electronic system can be easily calculated since the phononic action is quadratic in the displacement field whereas the electron-phonon interaction is a linear function of the lattice displacement (multiplied by the electronic staggered charge density). Integrating the displacement fields, in the integrals for the partition function, one gets in addition to (3), an effective interaction between the staggered components of the electronic charge densities (see for instance [9])

$$S_{\text{int}} = -2\pi v_c \lambda_l \int d\tau d\tau' dx \left\{ \sum_{l=1,2} \int d^2x d\tau' \rho^*(2lk_F, x, \tau') \left[\delta(\tau' - \tau) + \frac{1}{2\omega_l} \partial_\tau^2 e^{-\omega_l |\tau' - \tau|} \right] \rho(2lk_F, x, \tau) \right\}. \quad (5)$$

where

$$\rho(2k_F, x) = \sum_\sigma R_\sigma^\dagger(x) L_\sigma(x) = a_c \exp \left\{ i\sqrt{2\pi} \Phi_c(x) + 2ik_F x \right\} \cos \left\{ \sqrt{2\pi} \Phi_s(x) \right\} \quad , \quad (6)$$

$$\rho(4k_F, x) = a_u \exp \left\{ i\sqrt{8\pi} \Phi_c(x) + 4ik_F x \right\} \quad , \quad (7)$$

are the $2k_F$ and $4k_F$ -components of the staggered charge density end $\omega_l = \omega(2lk_F)$ for $l = 1, 2$ are the phonon frequencies and $\lambda_l = [\kappa \sin(lk_F a)]^2 / (\pi v_c \rho_l \omega_l^2 a^2)$, where ρ_l is the effective mass of the l -th mode. It is of course known [and can be seen also in the above formula (5)] that the electron-electron interaction mediated through phonons is constituted of two kinds of interactions. First there is an instantaneus attraction effect between the electronic staggered charge densities. By observing the formulae for the charge densities Eqs. (6-7) one can see that only the $2k_F$ component gives a contribution to the instantaneus component of the interaction. The $4k_F$ component of the staggered charge density have the particular exponential form of complex argument and does not give any contribution. Quantitatively the effect of the instanteneous attraction between the $2k_F$ components of the staggered charge density can be evaluated using the identity [10]. This shows that this kind of interaction renormalizes the LL parameters of both the charge and the spin channels. In the latter the additional constant will be with positive sign and will tend to increase g_s^0 to a value which we will assume to be still negative. A positive g_s will lead to a gap in the spin sector, something we are not undertaking to examine here.

The contribution from the nonlocal term, or the retarded attraction between the staggered charge densities, will be discussed a bit longer in the following since they are the factor that leads to the frequency dependence of the Luttinger liquid parameter K_c in the charge sector. Let us see first the effect of the interaction between the $4k_F$ components of the staggered charge density:

$$\begin{aligned}
& \int dx d\tau' : \rho(4k_F, x, \tau) : \left(\frac{\pi v_c \lambda_2}{2\omega_2} \partial_\tau^2 e^{-\omega_2 |\tau - \tau'|} \right) : \rho(-4k_F, x, \tau') : \\
&= - \int dx d\tau' : \partial_\tau \rho(4k_F, x, \tau) : : \partial_{\tau'} \rho(-4k_F, x, \tau') : \frac{\pi v_c \lambda_2}{2\omega_2} e^{-\omega_2 |\tau - \tau'|} \\
&= -4\pi^2 v_c a_u^2 \frac{\lambda_2}{\omega_2} \partial_\tau \Phi_c(\tau) \int d\tau' e^{-\omega_2 |\tau'|} \exp\{\mathrm{i}\sqrt{8\pi}[\Phi_c(\tau) - \Phi_c(\tau - \tau')]\} \partial_{\tau'} \Phi_c(\tau - \tau') \quad .
\end{aligned}$$

If we note with

$$\bar{f}_{4k_F}(\tau') = 4\pi^2 v_c a_u^2 \frac{\lambda_2}{\omega_2} e^{-\omega_2 |\tau'|} \langle e^{\mathrm{i}\sqrt{8\pi}\Phi_c(\tau)} e^{-\mathrm{i}\sqrt{8\pi}\Phi_c(\tau - \tau')} \rangle \quad , \quad F_{4k_F}(\tau) = \int d\tau' \bar{f}_{4k_F}(\tau') \Phi_c(\tau - \tau') \quad , \quad (8)$$

in the following we make the mean field approximation by representing the $4k_F$ contribution in ω -space in the following form

$$\int d\tau [\partial_\tau \Phi_c(\tau)] [\partial_\tau F_{4k_F}(\tau)] = \int d\omega \omega^2 \Phi_c(-\omega) F_{4k_F}(\omega) = \int d\omega \omega^2 \Phi_c(-\omega) \bar{f}_{4k_F}(\omega) \Phi_c(\omega) \quad . \quad (9)$$

The $2k_F$ components give for \bar{f}_{2k_F} two terms from which, within this approximation, only one gives a finite contribution in the dynamics. The first one being

$$\bar{f}_{1,2k_F}(\tau') = \pi^2 v_c a_c^2 \frac{\lambda_1}{\omega_1} e^{-\omega_1 |\tau'|} \langle e^{\mathrm{i}\sqrt{2\pi}\Phi_c(\tau)} e^{-\mathrm{i}\sqrt{2\pi}\Phi_c(\tau - \tau')} \cos[\sqrt{2\pi}\Phi_s(\tau)] \cos[\sqrt{2\pi}\Phi_s(\tau - \tau')] \rangle \quad . \quad (10)$$

is similar to \bar{f}_{4k_F} . The additional one is

$$\bar{f}_{2,2k_F}(\tau') = \pi^2 v_c a_c^2 \frac{\lambda_1}{\omega_1} e^{-\omega_1 |\tau'|} \langle e^{\mathrm{i}\sqrt{2\pi}\Phi_c(\tau)} e^{-\mathrm{i}\sqrt{2\pi}\Phi_c(\tau - \tau')} \rangle \quad (11)$$

multiplying

$$\partial_\tau \cos[\sqrt{2\pi}\Phi_s(\tau)] \partial_\tau \cos[\sqrt{2\pi}\Phi_s(\tau - \tau')] \quad . \quad (12)$$

In ω -space the term (10) will give a contribution similar to (9), namely

$$\int d\tau [\partial_\tau \Phi_c(\tau)] [\partial_\tau F_{1,2k_F}(\tau)] = \int d\omega \omega^2 \Phi_c(-\omega) \bar{f}_{1,2k_F}(\omega) \Phi_c(\omega) \quad , \quad (13)$$

whereas the term (11) can be shown to be a total time derivative and therefore we do not add it as a contribution.

In the contributing terms \bar{f}_{4k_F} and $\bar{f}_{2,2k_F}$ we have made the mean field approximations

$$\exp\{\mathrm{i}\sqrt{8\pi}[\Phi_c(\tau) - \Phi_c(\tau - \tau')]\} \approx \langle \exp\{\mathrm{i}\sqrt{8\pi}[\Phi_c(\tau) - \Phi_c(\tau - \tau')]\} \rangle = \left(\frac{\tau_0}{|\tau'|} \right)^{2d_{4k_F}} \quad (14)$$

and

$$\begin{aligned}
& \exp\{\mathrm{i}\sqrt{2\pi}[\Phi_c(\tau) - \Phi_c(\tau - \tau')]\} \cos[\sqrt{2\pi}\Phi_c(\tau)] \cos[\sqrt{2\pi}\Phi_c(\tau - \tau')] \approx \\
& \langle \exp\{\mathrm{i}\sqrt{2\pi}[\Phi_c(\tau) - \Phi_c(\tau - \tau')]\} \rangle \langle \cos[\sqrt{2\pi}\Phi_c(\tau)] \cos[\sqrt{2\pi}\Phi_c(\tau - \tau')] \rangle \sim \left(\frac{\tau_0}{|\tau'|} \right)^{2d_{2k_F}} \left(\frac{\tau_0}{|\tau'|} \right)^{2d_s} \quad ,
\end{aligned} \quad (15)$$

where $d_{4k_F} = 2K_c^0$ and $d_{2k_F} = K_c^0/2$, $d_s = 1/2$ and

$$\int_{-\infty}^{+\infty} d\tau' e^{-\omega_2 |\tau'|} \left(\frac{\tau_0}{\tau'} \right)^{4K_c^0} \approx \frac{2\tau_0}{4K_c^0 - 1} \quad . \quad (16)$$

τ_0 is a low cut-off of the order of ϵ_F^{-1} . The integral (16) is always positive since in the Hubbard model K_c^0 takes values decreasing from 1 to 1/2 as $u=U/t$ increases from 0 to ∞ (see for instance Frahm and Korepin [11]).

In ω -space the effect of the nonlocal term of (5) is that the charge sector can be described by the modified Gaussian action with the kinetic energy nonlocal in time:

$$S = \frac{1}{2K_c^0} \sum_{\omega, q} \Phi_c(-\omega, -q) \left[\frac{1}{v_c} \omega^2 f(\omega) + v_c q^2 \right] \Phi_c(\omega, q) , \quad f(\omega) = 1 + v_c K_c^0 \left[\bar{f}_{1,2k_F}(\omega) + \bar{f}_{4k_F}(\omega) \right] , \quad (17)$$

where the function $f(\omega)$ takes values between

$$f(\omega \gg 0) := 1 + v_c K_c^0 \int d\tau' [\bar{f}_{1,2k_F}(\tau') + \bar{f}_{4k_F}(\tau')] = 1 + 2\pi v_c^2 K_c^0 \tau_0 \left\{ a_c^2 \frac{\lambda_1}{\omega_1} + 4a_u^2 \frac{\lambda_2 K_c^0}{\omega_2(4K_c^0 - 1)} \right\} = k^2 \quad (18)$$

and $f(\omega \gg 0) := 1$. In Eq. (18) we introduced the ω -independent constant k .

It is interesting to explore the consequences of frequency dependence of $f(\omega)$. Its form, within our approximation, is given by

$$f(\omega) = 1 + \frac{\omega_0^2}{\omega^2 + \omega_0^2} (k^2 - 1) , \quad (19)$$

where $f(0) = k^2$ (the parameter k takes large values) and $f(\omega \gg 0) = 1$. ω_0 is considered to be the phonon's frequency (the phonons are considered as without dispersion and we can approximate $\omega_{2k_F} \approx \omega_{4k_F} = \omega_0$). Large values of k notify strong renormalization, and this is stronger at smaller frequencies (but not smaller than the critical one set from the spin sectors requirement of no gap opening). The value of the constant k is expected to be big, and experimental observations in materials like $K_{0.3}\text{MoO}_3$ [3] give a value of several hundred.

In time representation the action on the charge sector has the following form

$$S = \int dx d\tau \left\{ \frac{1}{2K_c^0} \left[\frac{1}{v_c} (\partial_\tau \Phi_c)^2 + v_c (\partial_x \Phi_c)^2 \right] + \partial_\tau \Phi_c(\tau) \int d\tau' [\bar{f}_{1,2k_F}(\tau') + \bar{f}_{4k_F}(\tau')] \partial_\tau \Phi_c(\tau - \tau') \right\} . \quad (20)$$

The effective retarded attraction between the staggered components of the charge density affects only the charge sector. In the spin sector K_s^0 remains 1, [preserving the SU(2) symmetry].

For the special limit $\omega = 0$ in $f(\omega)$ of (17), it takes the following form

$$S = \frac{1}{2K_c^0} \int dx d\tau \left[\frac{1}{v_c} k^2 (\partial_\tau \Phi_c)^2 + v_c (\partial_x \Phi_c)^2 \right] , \quad [f(\omega = 0)] , \quad (21)$$

which in the canonical form (4) is described by the new renormalized parameters

$$K_c = \frac{1}{k} K_c^0 , \quad \tilde{v}_c = \frac{1}{k} v_c . \quad (22)$$

The limit $\omega \gg 0$ in the charge sector is described by the action

$$S = \frac{1}{2K_c^0} \int dx d\tau \left[\frac{1}{v_c} (\partial_\tau \Phi_c)^2 + v_c (\partial_x \Phi_c)^2 \right] , \quad [f(\omega \gg 0)] . \quad (23)$$

We consider the case of K_c^0 being near 1 and neglect the renormalization coming from the local term, which is of the same magnitude as the renormalization of the spin sector and which we considered to be small. In this case $K_c = 1/k$.

The single-particle Green's function is expressed as a correlator of the chiral exponents of the charge and spin fields:

$$\begin{aligned} G(\tau, x) &= \langle \exp [i\sqrt{2\pi} \phi_c(\tau, x)] \exp [i\sqrt{2\pi} \phi_s(\tau, x)] \cdot \exp [i\sqrt{2\pi} \phi_c(0, 0)] \exp [i\sqrt{2\pi} \phi_s(0, 0)] \rangle \\ &= (\tau - x/v_s)^{-1/2} \langle \exp [i\sqrt{2\pi} \phi_c(\tau, x)] \exp [i\sqrt{2\pi} \phi_c(0, 0)] \rangle \end{aligned} \quad (24)$$

The model (17) leads to the Matsubara Green's function

$$G(x = 0; \tau) = \frac{1}{\tau} \exp \left\{ -\frac{1}{2} \int_0^{\epsilon_F/\omega_0} \frac{dx}{x} \left[\left(\frac{x^2 + 1}{x^2 + k^2} \right)^{1/4} - \left(\frac{x^2 + k^2}{x^2 + 1} \right)^{1/4} \right]^2 \sin^2(\omega_0 \tau x / 2) \right\} . \quad (25)$$

This Green's function for large τ behaves as

$$G(\tau) \xrightarrow{\tau \rightarrow +\infty} \frac{1}{\tau^{\theta_c+1}} \implies \rho_{\text{DOS}}(\omega) \xrightarrow{\omega \rightarrow 0^+} \omega_c^\theta ; \quad \theta_c = \frac{1}{4} \left(\frac{1}{\sqrt{K_c}} - \sqrt{K_c} \right)^2 ; \quad [f(\omega = 0)] , \quad (26)$$

which corresponds to $f(\omega = 0)$, Eq. (21). This is so because the exponential of the Green's function Eq. (26) for large τ behaves as $-[(\sqrt{k} - 1/\sqrt{k})^2/4] \ln \tau$.

For small τ , it bahaves as

$$G(\tau) \sim \frac{1}{\tau} \implies \rho_{\text{DOS}}(\omega) \xrightarrow{\omega \gg 0} \text{const} , \quad (\tau \rightarrow 0) ; \quad [f(\omega \gg 0)] , \quad (27)$$

corresponding to the case with $f(\omega)$ with large ω , Eq. (23), [if $G(\tau) \sim 1/\tau$ were in all τ space then $\tilde{G}(i\omega_n) = -2i \int_0^{+\infty} d\tau \sin(\omega_n \tau)/\tau = -2i \text{Si}(+\infty) = -i\pi$ and $\rho_{\text{DOS}}(\omega) = (-1/\pi) \Im m G^R = 1$].

To extract DOS on the whole frequency space one has to Fourier transform this function to get $\tilde{G}(i\omega_n)$ and then take the analytic continuation $i\omega_n \rightarrow \omega + i0$. The values of $\rho_{\text{DOS}}(\omega)$ between the two asymptotic limits, $\omega \rightarrow 0^+$ and $\omega \gg 0$, are shown in Fig 1. They are obtained numerically by analytic continuation of $\tilde{G}(i\omega_n)$ from the imaginary axis to just above the real axis. A remarkable feature of DOS is the peak at $\omega \approx K^{-1}\omega_0/2$ (see Fig. 2).

Since DOS is invariant under $K \rightarrow K^{-1}$ this empirical formula can be generalized as

$$\omega_{\text{peak}} = \frac{1}{2}(K^{-1} + K)\omega_0 . \quad (28)$$

It is interesting that the peak always occurs at frequencies larger than the characteristic phonon frequency ω_0 . At small (large) values of K this discrepancy can be quite substantial. For example, a peak in DOS has been observed in $\text{K}_{0.3}\text{MoO}_3$ at $\omega \approx 300$ meV. The behavior of DOS at smaller frequencies is almost linear in ω which suggests $K \approx 0.15$. Then Eq. (28) gives a reasonable estimate for the phonon frequency: $\omega_0 \approx 90$ meV.

For smaller ω_0 the Luttinger parameter K_c becomes small, the exponent θ_c becomes large and the peak approaches the origin. This is also observed in the numerical plots, and is in accord with (28).

The Fig. 1 clearly show also the crossover from the Luttinger-liquid type behavior with singular $d\rho/d\omega$ at $K > 0.17$ to the power-low suppressed with exponent larger than 1 behavior at $K < 0.17$.

To summarize, we have investigated in this paper the single particle density of states at the fermi level of 1D conductors at incommensurate fillings with electron-phonon interactions. The problem is studied using the Tomonaga-Luttinger liquid approch. The phonon degrees of freedom were integrated out and the remaining effective electron-electron interactions were studied. The electron-phonon interactions with large momentum transfer of $q \approx 2k_F$ and $q \approx 4k_F$ result in retardation effects which lead to the unusual form of LL model, namely with parameters of the charge sector depending on the frequency. The LL constant K is also a function of ω_0 , the phonon frequency. At small frequencies K_c and v_c are strongly renormalized by the interactions. We found the imaginary time Matsubara Green's function for this model and built the single particle density of states. Dos exhibits a peak which is proportional with the phonon frequency, but nevertheless they do not coincide.

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